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The research described below was carried out during the period 1 February 1998 to 30 September 2001. We have made significant progress on several fronts. We have obtained positive-weight quadrature rules that are exact for spherical harmonics of prescrided order mid that allow function evaluations at scattered points, and we have given algorithms for obtaining these weights. Based on these rules, we were able to construct neural networks for spheres using zonal activation functions. We also made progress on the difficult problem of locating multiple sources with neural networks. On another front, we provided error estimates for interpolating less smooth functions via networks with smooth activation functions; this is the first result of its kind. In addition, we provided a class of functions to which our error estimates aplly; these functions are both easy to use and locally supported, so that interpolation matrices arising from them will be banded.

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"Surface-Fitting and Analysis of Scattered Data via Radial and Related Basis Functions with Applications to Neural Networks"

Period: 1 February 1998—30 September 2001

by

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Summary

The research described below was carried out during the period 1 February 1998 to 30 September 2001. We have made significant progress on several fronts. We have obtained positive-weight quadrature rules that are exact for spherical harmonics of prescrided order and that allow function evaluations at scattered points, and we have given algorithms for obtaining these weights. Based on these rules, we were able to construct neural networks for spheres using zonal activation functions. We also made progress on the difficult problem of locating multiple sources with neural networks. On another front, we provided error estimates for interpolating less smooth functions via networks with smooth activation functions; this is the first result of its kind. In addition, we provided a class of functions to which our error estimates aplly; these functions are both easy to use and locally supported, so that interpolation matrices arising from them will be banded.

1 Review of Research

The research described below was carried out during the period 1 February 1998 to 30 September 2001, the final year being a no-cost extension. The work itself is communicated in the papers and informal technical reports listed in §2.

Publications are denoted by 'P', technical reports by 'T'. The numbering is from the lists in §2.1 and §2.2. Our research fits into the broad categories described below.

1.1 Error estimates and positive-weight quadrature

Our research on error estimates for generalized Hermite interpolation using radial-like basis functions on non-traditional spaces – the n-sphere, n-torus, and Riemannian manifolds – began with work done jointly with N. Dyn that is described in [P2]. These rates were the first for such manifolds, and made use of variational techniques in a reproducing kernel Hilbert space setting. For the sphere, these results depended on a sampling theorem for the sphere introduced by Driscoll and Healy [2]. The use of this sampling theorem limited the applicability of these results to the latitude-longitude grid on the sphere. At the time, one of our goals was to expand the range of applicability of this method. How we did this is described below.

We also completed joint work with R. Schaback [P12] investigating a version of a multilevel method introduced by Floater and Iske [1] that interpolates residuals, but uses convolutions of RBFs rather than the scaled RBFs employed in [1]. The methods employed were based on ones used in [P2]. We obtained rates of approximation for this interpolation process. These estimates were the first ever for cases in which parameters, such as spreads and actual basis functions, were allowed to change.

Building on the framework established by Dyn, Narcowich, and Ward in [P2], and joint with Professors Jetter and Stoeckler, we obtained rates of approximation by spherical-basis-function (SBF) interpolants for the case of scattered-data on the d-sphere [P3]. The work introduced the Banach-space idea of norming sets to surface fitting problems. The bounds obtained were explicit, in terms of the mesh norm of the data. In addition, new quadrature formulas, based on scattered-data, were provided for the sphere in [P4], but, unfortunately, these gave no control on the weights in the quadrature formulas.

This lead to a deeper investigation of the possibility of obtaining positive weight, scattered-data quadrature formulas for the d-sphere. These formulas would reproduce spherical harmonics of a given order, but at the same time use a number of points from the scatted data comparable to the dimensions of the spaces of spherical harmonics involved. Such results, which are well known and have long been utilized for special point sets in intervals on the line and in rectangular boxes in higher dimensions, were not known for the sphere. In [P6], which was joint with H. Mhaskar, we not only obtained such formulas, but we arrived at them by establishing an important norm equivalence. We showed that, for the space of spherical harmonics on S^d having order n or less, the $L^p(S^d)$ norm is equivalent to the discrete ℓ^p norm of the spherical harmonics restricted to a point set $X \in S^d$, where the number of points in X is comparable to the dimension of the space of spherical harmonics. This generalizes to the sphere an old result of Marcinkiewicz and Zygmund for trigonometric polynomials. One spinoff of the norming-set technique is a scattered-data positive weight quadrature formula on a cube in R^d and related approximation results; these were reported in [P8]. Another concerns neural networks, which we will describe in §1.2 below.

Others applications of norming sets again deal with error estimates. RBF error estimates on compact domains in R^d were first obtained for thin-plate splines by Duchon [3, 4] and for RBFs in general by Madych and Nelson [5, 6]. Recently, Wendland [14] pointed out that the unevaluated constants in these papers can be estimated using norming sets, and did so for the Gaussian RBF. In joint work with Wendand [T2] we employed the norming set technique to provide new and refined error estimates that apply to scattered-data interpolants and their derivatives, not only in R^dbu t on the d-torus and 2-sphere as well. In many cases our estimates provide bounds orders of magnitude smaller than those previously known.

Many of the results mentioned above dealt with error estimates occurring when the functions sampled belong to the reproducing kernel Hilbert space induced by an RBF or similar kernel. These spaces are often called *native spaces*. The overall effect is that these results are limited to having the functions sampled be as a smooth as the RBF, itself. In many cases this is not a problem. However, when the smoothness class of a target function is unknown, this does become a problem.

In work done jointly with R. Schaback, we began addressing this problem. We showed in [P13] that we could *approximate* target functions outside of the native space using linear combinations of RBFs. The linear process we provided in that paper, while yielding good results, is difficult to implement. We felt we could do better.

The key to doing better is a technique "dual" to the one employing norming sets; it was presented in [P10]. This technique, which is functional analytic in character, allows one to obtain simultaneous interpolation and a near-optimal degree of approximation by radial and related basis functions, for a cube, torus or 2-sphere. Related results are also found in [T3].

Our most recent work [T5] applies the "dual" norming set technique to obtain Sobolev-type error estimates for interpolating functions $f \in C^{2k}(S^d)$ from "shifts" of a smoother SBF defined on S^d. Moreover, these estimates are close to the optimal approximation order, and obtaining them is computationally feasible. Although RBF interpolation has been in in use for nearly a score of years, no previous work has successfully shown that RBF-type interpolants converge when the sampled function is not in the native space. This is the first paper to do so.

1.2 Neural networks and PDEs

The field of neural networks encompasses a vast area, overlaps with many others fields, and can be approached in a variety of ways. Our approach is that of Poggio and Girosi [9], who view *learning* as a problem of *hypersurface reconstruction*. In a broad sense, all of the work we have done has been aimed at this problem. Even so, we wish to discuss results that specifically apply to neural networks, especially ones on non-traditional spaces – spheres and other manifolds.

Neural networks on spheres come up in applications to geophysical problems. Networks on other spaces that we've studied arise in connection with neural beamforming problems [8, 11]. Our paper [P15], joint with O'Donnell and Southall, details our work in attacking the problem of direction finding in the presence of multiple sources and sets out new avenues for future research. Concerning the sphere, we have written several papers addressing questions concerning stability, interpolation, and approximation with networks using zonal functions as activation functions for the network. In [P14], we obtain stability estimates–i.e., norms of inverses of interpolation matrices and condition numbers for these matrices. More recently, we employed the quadrature formulas from [P6] to study approximation power for zonal function networks; these results, which are reported in [P5], showed that the networks themselves have nearly optimal Sobolev-type approximation properties. In [P9] and [T4], we construct a multiresolution analysis of the standard Hilbert space on a Euclidean sphere, which can be implemented directly by neural networks. The neural networks may utilize any sufficiently smooth function as an activation function, and their size can be determined in advance. We introduce frame operators that can analyze data selected at scattered sites. These frames can be used to detect singularities, even in higher order derivatives.

Papers dealing with applications of RBFs to solving PDEs numerically have for the most part been experimental. Definite theoretical results on error estimates and stability have been looked at in very few cases, and then only for elliptic problems, which can be solved via finite element methods. In joint work with R. Lorentz [T1], we present RBF/Hermite collocation methods that are adaptive, highly flexible, multivariate, and can be employed in non-traditional spaces, the sphere for example. We analyze in detail a simple transport problem solved via such a method, and we found that it provides spectral convergence orders that are competitive with previously known polynomial methods, which have very limited scope and are not adaptive. This raises important questions for future work.

1.3 Locally supported basis functions

To describe the results that we have gotten, we need to provide some background material. A positive definite function on a sphere is a function $\phi(\cos\theta)$, where θ is the geodesic (great circle) distance between two points on a sphere. The idea is that the interpolation matrices with entries $\phi(\cos\theta_{j,k})$ are positive semi-definite for an arbitrary finite set of scattered points on the sphere. Long ago Schoenberg [10] characterized such functions as being those having Legendre expansions,

$$\phi(\cos\theta) = \sum_{\ell=0}^{\infty} a_\ell P_\ell(\cos\theta),$$

in which $a_\ell \geq 0$ and $P_\ell(\cos\theta)$ is the ℓ^{th} degree Legendre polynomial corresponding to the n-sphere. When $n = 2$, these are the standard, familiar Legendre polynomials. When $n \neq 2$, they are proportional to Gegenbauer polynomials [7]. To guarantee that the interpolation matrices associated with ϕ are positive definite and thus are invertible, we impose the condition that $a_\ell > 0$ for all ℓ. A ϕ satisfying this is a *spherical basis function* (SBF).

There are three ways of obtaining SBFs: (1) directly from the series; (2) from functions having known expansions, such as $e^{\cos\theta}$ or a generating function; and, finally, (3) from restricting RBFs on Euclidean spaces to a sphere. The difficulty with (1) is that either one has to sum an infinite series or obtain good numerical approximations to its sum. Most of the SBFs that we have came by way of (2). Somewhere along the line a series expansion for a function was known, and the coefficients were observed to be strictly positive.

Restricting RBFs to the sphere is simple enough. Suppose that $x, y \in S^n$ and that the angle between x and y is θ, so that the Euclidean dot product $x \cdot y = \cos\theta$. If we let Φ be an RBF in R^{n+1}, then

$$\phi(x \cdot y) := \Phi(\|x - y\|_2)|_{x,y \in S^n}$$

is easily seen to be positive definite on S^n. The hard problem was determining whether or not whether or not a ϕ gotten in this way was an SBF–that is, whether or not all its Legendre coefficients were strictly positive. In [T5], we showed that under very mild conditions, such ϕ were SBFs. This opened the door to introducing a new class of SBFs; these are locally supported functions arising via restrictions of Wendland's compactly supported RBFs [12, 13]. These new functions are quite attractive; they can be both explicitly and easily computed and are also have good convergence properties. Future work would involve further exploration of their properties and fast evaluation methods.

2 Publications, Reports, and Talks

2.1 Publications

1. F. Deutsch, W. Li, and J. D. Ward, Best approximation from the intersection of a closed convex set and a polyhedron in Hilbert space, weak Slater conditions, the strong conical hull intersection property, SIAM J. Optimiz. Th., 10 (1999), 252-268.

2. N. Dyn, F. J. Narcowich and J. D. Ward, Variational Principles and Sobolev-Type Estimates for Generalized Interpolation on a Riemannian Manifold, Constructive Approximation, 15 (1999) 175-208.

3. K. Jetter, J. Stoeckler, and J. D. Ward, Error estimates for scattered data interpolation on spheres, Math. Comp., 68 (1999), 733-747.

4. K. Jetter, J. Stoeckler, and J. D. Ward, " Norming sets and spherical cubature formulas," in: Advances in Computational Mathematics, Z. Chen,

Y. Li, C. A. Micchelli and Y. Xu (eds.), Macel Dekker, Inc, New York, 1999, pp. 237-244.

5. H. N. Mhaskar, F. J. Narcowich, and J. D. Ward, Approximation Properties of Zonal Function Networks Using Scattered Data on the Sphere, Adv. Comput. Math., 11 (1999), 121-137.

6. H. N. Mhaskar, F. J. Narcowich, and J. D. Ward, Spherical Marcinkiewicz-Zygmund Inequalities and Positive Quadrature, Math. Comp., **70** (2001), 1113-1130.

7. H. N. Mhaskar, F. J. Narcowich, and J. D. Ward, "Representing and Analyzing Scattered Data on Spheres," Multivariate Approximation and Applications, edited by N. Dyn, D. Leviaton, D. Levin, and A. Pinkus, Cambridge University Press, Cambridge, U. K., 2001.

8. H. N. Mhaskar, F. J. Narcowich, and J. D. Ward, Quasi-interpolation in shift invariant spaces, J. Math. Anal. Appl., **251** (2000), 356-363.

9. H. N. Mhaskar, F. J. Narcowich, J. Prestin, and J. D. Ward, Polynomial frames on the sphere, Adv. Compt. Math., to appear.

10. H. N. Mhaskar, F. J. Narcowich, N. Sivakumar, and J. D. Ward, Approximation with Interpolatory Constraints, Proc. AMS, to appear.

11. F. J. Narcowich, "Recent Developments in Approximation via Positive Definite Functions," in Approximation Theory IX, Volume 2: Computational Aspects, C. K. Chui and L. Schumaker (eds.), Vanderbilt University Press, Nashville, TN, 1998, pp. 221-242.

12. F. J. Narcowich, R. Schaback, and J. D. Ward, Multilevel Interpolation and Approximation, Applied and Computational Harmonic Analysis, 7 (1999), 243-261.

13. F. J. Narcowich, R. Schaback and J. D. Ward, Approximation in Sobolev Spaces by Kernel Expansions, J. Approx. Theory, to appear.

14. F. J. Narcowich, N. Sivakumar, and J. D. Ward, Stability results for scattered-data interpolation on Euclidean spheres, Advances in Computational Mathematics 8 (1998) 137-163.

15. T. H. O'Donnell, F. J. Narcowich, H. L. Southall, and J. D. Ward, "Multiple source direction finding with reduced training and increased generalization," in Proceedings of the Millennium Conference on Antennas & Propagation, held from 9 - 14 April 2000, Davos, Switzerland, Publication no. SP-444, ESA Publications Division, ESTEC, 2200 AG Noordwijk.

2.2 Technical Reports

1. R. Lorentz, F. J. Narcowich, and J. D. Ward, Collocation Discretizations of the Transport Equation with Radial Basis Functions, preprint.
2. F. J. Narcowich, H. Wendland and J. D. Ward, Refined Error Estimates for Radial Basis Function Interpolation, preprint.
3. F. J. Narcowich, N. Sivakumar and J. D. Ward, On Convergent Interpolatory Processes Associated with Periodic Basis Functions, preprint.
4. H. N. Mhaskar, F. J. Narcowich, and J. D. Ward, Neural Network Frames on the sphere, preprint.
5. F. J. Narcowich and J. D. Ward, Scattered-Data Interpolation on Spheres: Error Estimates and Locally Supported Basis Functions, preprint.

2.3 Research Conference Talks

F. J. Narcowich

- Narcowich gave a plenary address at the 9TH INTERNATIONAL CONFERENCE ON APPROXIMATION THEORY, 3-6 January 1998, Vanderbilt University, Nashville, TN (C. Chui and L. Schumaker, organizers)
- Narcowich gave an invited half-hour talk, "Remarks on scattered-data surface fitting via positive definite kernels," EILAT98 International Conference on Multivariate Approximation and Interpolation with Applications in CAGD, Signal, and Image Processing, held 7-11 September 1998 in Eilat, Israel
- Narcowich gave an invited half-hour talk, "Scattered data quadrature for spheres," Session on Mathematical Methods of Geodesy at the Mathematiches Forschungsinstitut Oberwolfach, 29 March - 3 April 1999. The session was organized by W. Freeden, E. Grafarend, and L. Svensson.
- Narcowich gave an invited twenty-minute talk, "Multiple source direction finding with reduced training and increased generalization," at the Millennium Conference on Antennas & Propagation, held from 9 - 14 April 2000, Davos, Switzerland.
- Narcowich gave an invited twenty-minute talk, "Scattered Data Interpolation on Spheres: Locally Supported Basis Functions,"at the Special Session on Sphere Related Approximation and Applications, AMS Regional Meeting in Chattanooga, TN, October 5–6, 2001.

J. D. Ward

- Ward gave an invited, one-hour address at the conference on CADG AND WAVELETS held at Montecatini, Italy, 15-17 June 1998
- Ward gave an invited half-hour talk, "Remarks on qudrature formulas for the n-sphere," EILAT98 International Conference on Multivariate Approximation and Interpolation with Applications in CAGD, Signal, and Image Processing, held 7-11 September 1998 in Eilat, Israel
- Ward gave an invited one-hour talk, "Approximation from spaces of shifts of a positive definite kernel," International conference in Approximation Theory, held 28 Sept - 2 Oct in Dortmund, Germany
- Ward gave a one-hour invited talk, "Some remarks on wavelets on the m-sphere," given at the International Conference on Wavelet Analysis and Its Applications, held from 15 - 20 November 1999 at Zhongshan University, Guangzhou, P. R. China
- Ward gave a contributed talk, "Convergent interpolatory processes associated with periodic basis functions," at the symposium "Trends in Approximation Theory" held from 17 - 20 May 2000 at Vanderbilt University, Nashville, TN.
- Ward gave a contributed talk, "Approximation with interpolatory constraints," at the TENTTH INTERNATIONAL CONFERENCE ON APPROXIMATION THEORY, 26–29 March 2001, University of Missouri at St. Louis, St. Louis, MO (C. Chui and L. Schumaker, organizers).
- Ward gave an invited colloquim on Wednesday, November 13 at the University of Georgia, Athens, GA.
- Ward gave an invited twenty-minute talk, "Scattered Data Interpolation on Spheres: Approximating Rough functions by Smooth Kernels,"at the Special Session on Sphere Related Approximation and Applications, AMS Regional Meeting in Chattanooga, TN, October 5–6, 2001.

3 Activities

- Dr. Ward visited Major O'Donnell at Hanscomb AFB on 31 July 1998. He discussed a number of mathematical problems concerning location of multiple sources using neural networks and artificial arrays.
- Narcowich visited Terry O'Donnell at Hanscom from 17 May to 19 May 1999. The purpose of this visit was to discuss various aspects of detection of multiple sources via neural beamforming. The details of this visit were given in a report to Dr. Nachman, written on 24 May.

- Narcowich and Ward, and Robert Schaback, from Goettingen University in Germany, spent two weeks, 6 August 2000 - 19 August 2000, at the Mathematische Forschungsinstitut Oberwolfach, under the auspices of the Volkswagen-Stiftung "Research-in-Pairs" program. Professor Robert Schaback is a leader in the field of radial basis functions.
- Narcowich and Ward, along with H. Mhaskar, were asked by the organizers of the EILAT98 International Conference mentioned above to write a survey article to be appear in a book. The survey article that resulted is listed as [P7].
- Ward attended the CBMS lecture series on wavelets, from 22 - 26 May at the University of Missouri in St. Louis; David Donoho was principal speaker.
- Narcowich attended an IMA Workshop on Geometric Design, held from 23 April to 30 April 2001 at the University of Minnesota, and organized by L. Schumaker.

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